Simulation of Nuclear Flames in Type Ia Supernovae

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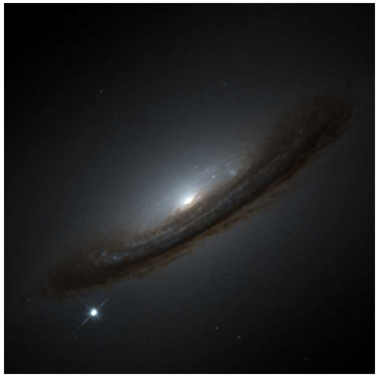
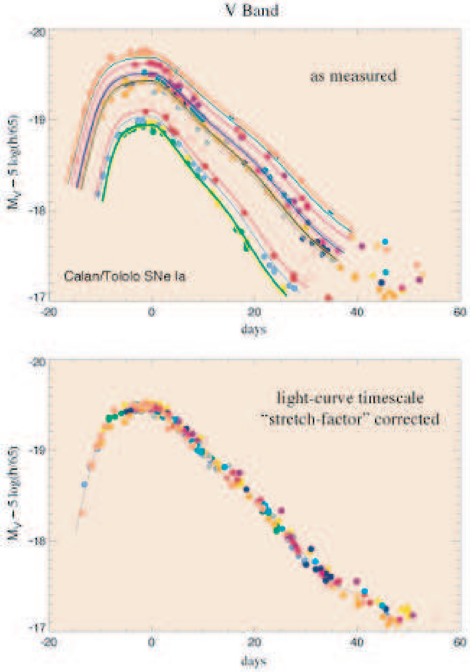
Type Ia Supernovae

- Brightness rivals that of host galaxy, L $\approx 10^{43}$ erg / s
- Large amounts of $^{56}\mathrm{NI}$ produced
  - Radioactivity powers the lightcurve
- Light curve is robust
  - Variations can be corrected for via a single parameter function.
- Thermonuclear explosion of C/O white dwarf.
  - Must begin as a deflagration
  - Considerable acceleration is required

Type Ia supernovae

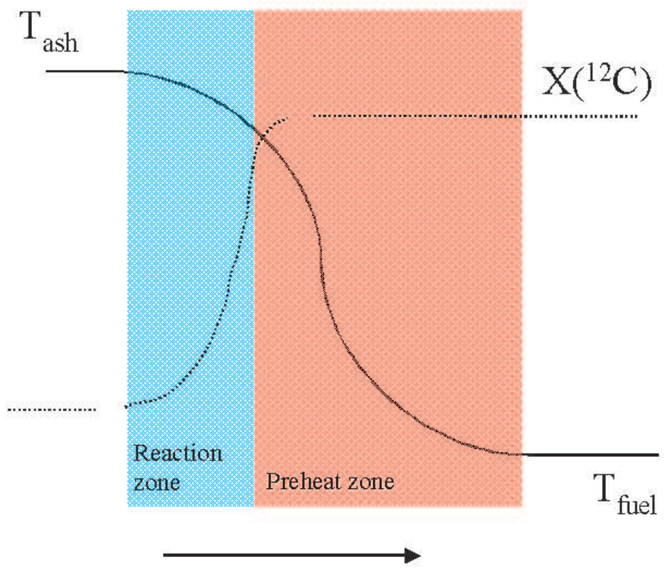




Flames

Begins as a deflagration

- Subsonic burning front
  - Pressure is continuous across the front
  - Density drops in the ash region.
- Thermal diffusion transports the heat



Laminar speed too slow

- Must accelerate considerably at low densities.
- May transition to detonation

SNe Ia Unstable Flames

Explosion begins as a flame in the interior of the white dwarf.

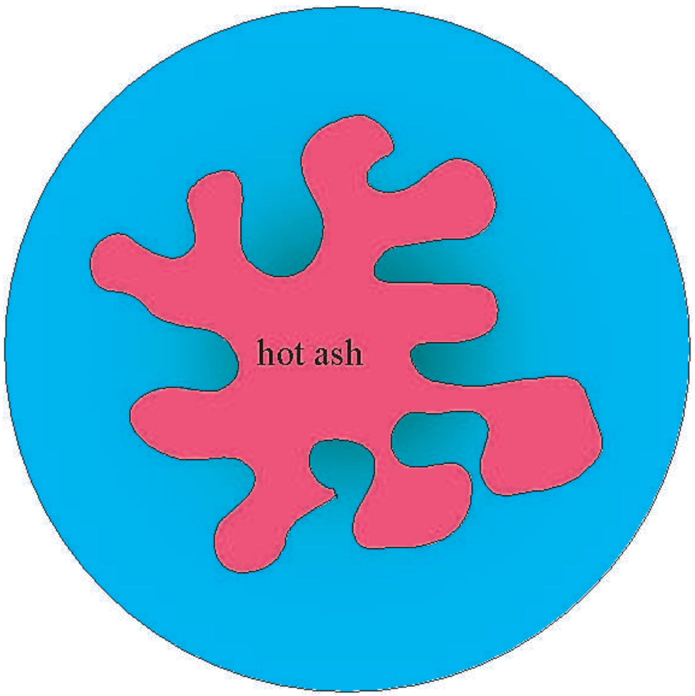
- $\approx$ 100 years of convection preceed ignition
- Subsonic propagation allows the star to expand.

Hot ash is less dense than the cool fuel.

Subjected to numerous instabilities.

What are the mechanisms for flame acceleration

Does the star detonate or is the supernovae purely a deflagration



Large Scale Simulations

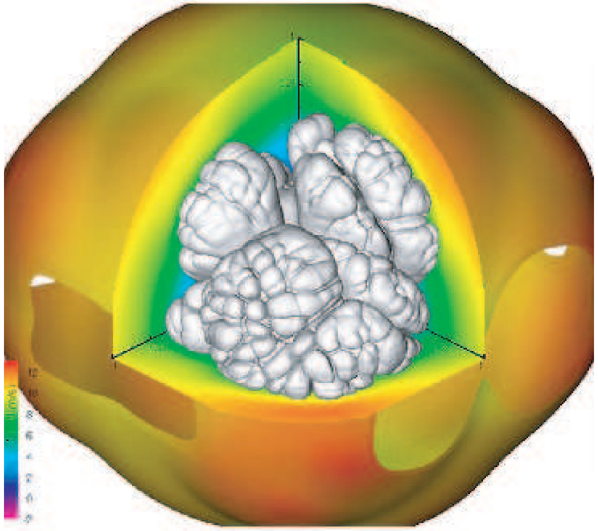
Instabilities are the dominant acceleration mechanism.

Pure deflagrations can unbind the star.

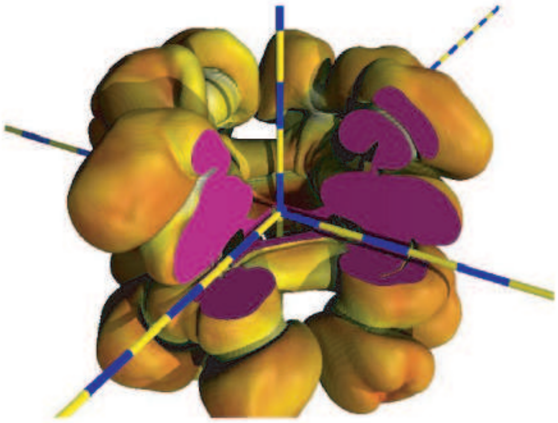
Some flame model is required.

- Stellar scale 10^8 cm
- Flame width 10^{-5} - 10 cm

Existing full-star simulations assume a turbulent flame speed



Gamezo et al. (2003)



Reinecke et al. (2003)

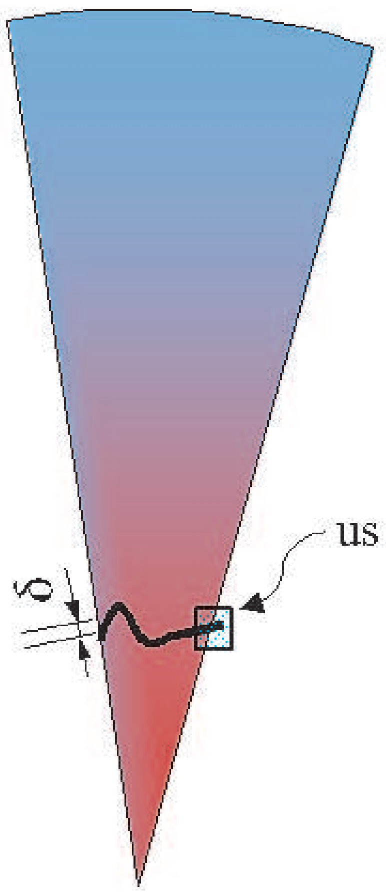
Nuclear flame microphysics

Our approach is to start with detailed flame physics

Resolve the thermal structure of the flame and work up to large scales

- Parameter free.
- Resolved calculations can be used to validate flame models.

Look for scaling relations that will act as subgrid models.



Type Ia Supernovae Characteristics

Ra $\approx 10^{25}$ – buoyancy to diffusion forces

- Nature of convection is not well known in this regime.

Re $\approx 10^{14}$ – inertial to viscous forces
Pr $\approx 10^{-4}$ – momentum transport to heat conduction

- Viscosity effects are unimportant.

Le $\approx 10^{7}$ – energy transport to mass transport

- Mass diffusion can be neglected.
- Large departure from typical Le $\approx$ 1 terristrial flames.

See Wunsch, Woosely and Kuhlen (2003)

Compressible flow equations

Compressible Navier-Stokes equations:

$$\rho_t + \nabla \cdot \rho U = 0$$

$$(\rho U)_t + \nabla \cdot (\rho U U + p) = \rho \vec{g} + \nabla \cdot \tau$$

$$(\rho E)_t + \nabla \cdot (\rho U E + U p) = \nabla \cdot \kappa \nabla T + \nabla \cdot \tau U$$

$$(\rho X_m)_t + \nabla \cdot \rho U X_m = \rho \dot{\omega}_m + \nabla \cdot \rho D \nabla X_m$$

ρ	density	T	temperature
X_m	mass fractions	$\vec{g}$	force of gravity
$\dot{\omega}_m$	production rate for X_m	p	pressure
u	flow velocity	$\mathcal{D}_m$	species diffusion coefficient
E	total energy	τ	stress tensor

Characterization of stellar material

Timmes equation of state provides:

$$e(\rho, T, X_k) = e_{ele} + e_{rad} + e_{ion} \qquad p(\rho, T, X_k) = p_{ele} + p_{rad} + p_{ion}$$

$$\begin{aligned} e_{ele} &= \text{fermi} \\ e_{rad} &= aT^4/\rho \\ e_{ion} &= \tfrac{3kT}{2m_p} \textstyle\sum_m X_k/A_m \end{aligned} \qquad \begin{aligned} p_{ele} &= \text{fermi} \\ p_{rad} &= aT^4/3 \\ p_{ion} &= \tfrac{\rho kT}{m_p} \textstyle\sum_m X_k/A_m \end{aligned}$$

Simulation strategy

Standard approach is to solve the compressible equations using a compressible adaptive mesh refinement algorithm

- Hillebrandt, Niemeyer et al. at MPI, Garching
- Oran et al. at NRL
- Rossner, Kokhlov, Plewa, et al. at U. Chicago

However, these flames are extremely low Mach number (< 0.1 %)

- Generalize low Mach number formulation to general equation of state
  - Eliminate acoustic time-step restriction while retaining compressibility effects due to heat release
  - Conserve species and enthalpy
- Projection formulation
- Adaptive mesh refinement
  - Localize mesh where needed
  - Refine in time and space
  - Complexity from synchronization

Asymptotics in Mach number

Combustion: Rehm & Baum 1978, Majda & Sethian 1985

Atmospheric flows: Durran 1989, Almgren, Botta, & Klein 1999

Start with the compressible Navier-Stokes equations for multicomponent reacting flow, and expand in the Mach number, $M = U/c$.

Asymptotic analysis shows that:

$$p(\vec{x}, t) = p_0 + \pi(\vec{x}, t) \quad \text{where} \quad \pi / p_0 \sim \mathcal{O}(M^2)$$

- p_0 does not affect local dynamics, π does not affect thermodynamics
- Acoustic waves analytically removed (or, have been “relaxed” away)

Low Mach Number Formulation

Low Mach number equations of motion

$$
\begin{aligned}
&\rho_t + \nabla \cdot \rho u = 0 \\
&(\rho X_m)_t + \nabla \cdot \rho u X_m = \rho \dot{\omega}_m \\
&(\rho u)_t + \nabla \cdot (\rho u u) + \nabla \pi = \rho \vec{g} \\
&(\rho h)_t + \nabla \cdot (\rho u h) = \nabla \cdot \kappa \nabla T
\end{aligned}
$$

ρ	density		
X_m	mass fractions	T	temperature
$\dot{\omega}_m$	production rate for X_m	$\vec{g}$	force of gravity
u	flow velocity	π	perturbational pressure
$h = e + p/\rho$	enthalpy		

Together with a constraint equation $p(\rho, T, X_m) = p_{\text{amb}}$

How do we solve this constrained system of PDE's.

Incompressible Navier Stokes Equations

For iso-thermal, single fluid systems this analysis leads to the incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

How do we develop efficient integration schemes for this type of constrained evolution system?

Vector field decomposition

$$V = U_d + \nabla \phi$$

where $\nabla \cdot U_d = 0$

and

$$\int U \cdot \nabla \phi dx = 0$$

We can define a projection $\mathbf{P}$

$$\mathbf{P} = I - \nabla(\Delta^{-1})\nabla \cdot$$

such that $U_d = \mathbf{P}V$

Solve

$$-\Delta \phi = \nabla \cdot V$$

Projection method

Incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla p = \mu \Delta U$$

$$\nabla \cdot U = 0$$

Projection method

Advection step

$$\frac{U^* - U^n}{\Delta t} + U \cdot \nabla U = {}^1\!/\!_2 \mu \Delta (U^* + U_n) - \pi^{n-{}^1\!/\!_2}$$

Projection step

$$U^{n+1} = \mathbf{P} U^*$$

Recasts system as initial value problem

$$U_t + \mathbf{P}(U \cdot \nabla U - \mu \Delta U) = 0$$

Combustion

How can this approach be generalized to low Mach number reacting flows?

- Finite amplitude density variations
- Compressiblility effects

Proposed extensions of the projection method fall into two basic classes:

Constant coefficient projection

- McMurtry, Riley, Metcalfe, AIAA J., 1986.
- Rutland & Fertziger, C&F, 1991.
- Zhang and Rutland, C&F, 1995.
- Cook and Riley, JCP, 1996.
- Najm, Trans. Phen. in Comb., 1996
- Najm & Wyckoff, C&F, 1997.
- Quian, Tryggvason & Law, JCP 1998.
- Najm, Knio & Wyckoff, JCP, 1998.

Variable coefficient projection

- Bell & Marcus, JCP, 1992.
- Lai, Bell, Colella, 11th AIAA CFD, 1993.
- Pember et al., Comb. Inst. WSS, 1995.
- Pember et al., Trans. Phen. Comb., 1996.
- Pember et al., CST, 1998.
- Schneider et al., JCP, 1999.
- Day & Bell, CTM, 2000.
- Nicoud, JCP, 2000.

Variable coefficient projection

Generalized vector field decomposition

$$V = U_d + \frac{1}{\rho}\nabla\phi$$

where $\nabla \cdot U_d = 0$ and $U_d \cdot n = 0$ on the boundary

Then U_d and $\frac{1}{\rho}\nabla\phi$ are orthogonal in a density weighted space.

$$\int \frac{1}{\rho}\nabla\phi \cdot U \; \rho \, dx = 0$$

Defines a projection $\mathbf{P}_\rho = I - \frac{1}{\rho}\nabla((\nabla \cdot \frac{1}{\rho}\nabla)^{-1})\nabla\cdot$ such that $\mathbf{P}_\rho V = U_d$.

$\mathbf{P}_\rho$ is idempotent and $||\mathbf{P}_\rho|| = 1$

Variable coefficient projection method

We can use this projection to define a projection scheme for the variable density system

$$\rho_t + \nabla \cdot \rho u = 0$$

$$U_t + U \cdot \nabla U + \frac{1}{\rho} \nabla \pi = 0$$

$$\nabla \cdot U = 0$$

Advection step

$$\rho^{n+1} = \rho^n - \Delta t \nabla \cdot \rho U$$

$$U^* = U^n - \Delta t\, U \nabla \cdot U - \frac{1}{\rho} \nabla \pi^{n-1/2}$$

Projection step

$$U^{n+1} = \mathbf{P}_\rho U_d$$

Recasts system as initial value problem

$$U_t + \mathbf{P}_\rho (U \cdot \nabla U) = 0$$

Combustion

$$\textbf{Momentum} \quad \frac{\nabla \rho u}{\nabla t} + \nabla \cdot (\rho u u) = -\nabla \pi + \nabla \cdot \tau$$

$$\textbf{Species} \quad \frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\rho u Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$$

$$\textbf{Mass} \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$

$$\textbf{Energy} \quad \frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \vec{u}) = \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$$

Differentiate the EOS, $p_0 = \rho \mathcal{R} T \sum_m \frac{Y_m}{W_m}$, along particle paths

$$0 = \frac{1}{\rho}\frac{D\rho}{Dt} + + \frac{1}{T}\frac{DT}{Dt} + \frac{\mathcal{R}}{R}\sum_m \frac{1}{W_m}\frac{DY_m}{Dt}$$

$$\nabla \cdot U = -\frac{1}{T}\frac{DT}{Dt} - \frac{\mathcal{R}}{R}\sum_m \frac{1}{W_m}\frac{DY_m}{Dt} \equiv S$$

In combustion $h = \Sigma h_m(T) Y_m$ so enthalpy equations give $\frac{DT}{Dt}$

Inhomogeneous constraints

We can use the variable-ρ projection to define a projection scheme for inhomogeneous constraints

$$U_t + U \cdot \nabla U + \frac{1}{\rho}\nabla \pi = \tau$$

$$\nabla \cdot U = S$$

Advection step

$$U^* = U^n - \Delta t \, U \nabla \cdot U = \Delta t \, \tau - \frac{1}{\rho}\nabla \pi^{n-1/2}$$

Projection step

$$U = U_d + \nabla \xi$$

where

$$\nabla \cdot \nabla \xi = S$$

$$U^{n+1} = \mathbf{P}_\rho (U^* - \nabla \xi) + \nabla \xi$$

$\nabla \cdot U$ Constraint

As in combustion p_0 is constant along particle paths.

$$p_0 = p(\rho, T, X_m)$$

$$\rho \frac{Dp_0}{Dt} = 0 = \rho \frac{\partial p}{\partial \rho} \frac{D\rho}{Dt} + \rho \frac{\partial p}{\partial T} \frac{DT}{Dt} + \rho \sum_m \frac{\partial p}{\partial X_m} \frac{DX_m}{Dt}$$

$$0 = -\rho^2 \frac{\partial p}{\partial \rho} \nabla \cdot u + \rho \frac{\partial p}{\partial T} \frac{DT}{Dt} + \rho \sum_m \frac{\partial p}{\partial X_m} \dot{\omega}_m$$

$$\nabla \cdot u = \frac{1}{\rho^2 \frac{\partial p}{\partial \rho}} \left(\rho \frac{\partial p}{\partial T} \frac{DT}{Dt} + \rho \sum_m \frac{\partial p}{\partial X_m} \dot{\omega}_m \right)$$

$\nabla \cdot U$ Constraint

In the supernovae context $h = h(\rho, T, X_m)$ but derivation of T equation must reflect constraint. Write

$$h = h(\rho(p, T, X_m), T, X_m)$$

Then

$$\rho \frac{Dh}{Dt} = \rho \frac{\partial h}{\partial T} \frac{DT}{Dt} + \rho \sum_m \frac{\partial h}{\partial X_m} \frac{DX_m}{Dt}$$

$$\rho c_p \frac{DT}{Dt} = \nabla \cdot \kappa \nabla T - \rho \sum_m \frac{\partial h}{\partial X_m} \dot{\omega}_m$$

Here $\frac{\partial h}{\partial T} = \frac{\partial h}{\partial \rho} \frac{\partial \rho}{\partial T} + \frac{\partial h}{\partial T}$

$$\nabla \cdot U = \frac{1}{\rho \frac{\partial p}{\partial \rho}} \left(\frac{1}{\rho c_p} \frac{\partial p}{\partial T} \left(\nabla \cdot \kappa \nabla T - \rho \sum_m \frac{\partial h}{\partial X_m} \dot{\omega}_m \right) + \sum_m \frac{\partial p}{\partial X_m} \dot{\omega}_m \right)$$

2nd Order Fractional Step Scheme

First Step:

Construct an intermediate velocity field U^*:

$$\frac{U^* - U^n}{\Delta t} = -[U^{ADV} \cdot \nabla U]^{n+\frac{1}{2}} - \frac{1}{\rho^{n+\frac{1}{2}}} \nabla \pi^{n-\frac{1}{2}} + \frac{1}{\rho^{n+\frac{1}{2}}} \frac{(\tau^n + \tau^*)}{2}$$

and advance species concentrations and enthalpy

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} = -\nabla \cdot (\rho U^{ADV})^{n+\frac{1}{2}}$$

$$\frac{\rho^{n+1}\chi^{n+1} - \rho^n \chi^n}{\Delta t} + \nabla \cdot (\rho U^{ADV} \chi)^{n+\frac{1}{2}} = D_\chi + R_\chi \quad for \ \chi = h, Y_m$$

Enforce the constraint

Use the updated values to compute S^{n+1}

Decompose $\vec{U}^{n+1,*}$ to extract the component satisfying the divergence constraint.

This decomposition is achieved by solving

$$\nabla \cdot \left(\frac{1}{\rho} \nabla \phi \right) = \nabla \cdot \vec{U}^{n+1,*} - S^{n+1}$$

for ϕ, and setting

$$\pi^{n+1/2} = \pi^{n-1/2} + \phi$$

and

$$\vec{U}^{n+1} = \vec{U}^{n+1,*} - \frac{1}{\rho} \nabla \phi$$

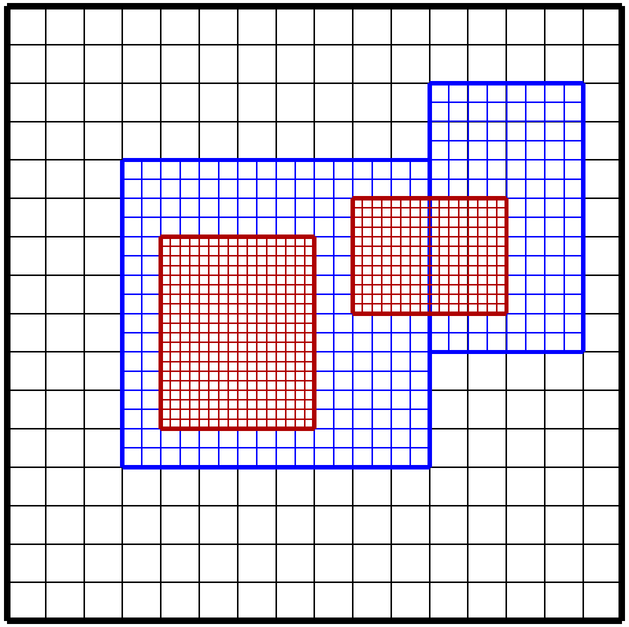
Exploits linearity to represent the compressible component of the velocity

AMR

Block-structured hierarchical grids

Each grid patch (2D or 3D)

- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed to track time-dependent features



2D adaptive grid hierarchy

Subcycling:

- Advance level ℓ, then
  - Advance level $\ell + 1$
    level ℓ supplies boundary data
  - Synchronize levels ℓ and $\ell + 1$

Computational Studies

Carbon, oxygen, magnesium flames

Single step reaction derived from Caughlan and Fowler

$$\dot{X}_{^{12}\mathrm{C}} = -\frac{\rho}{12} R(T) X^2_{^{12}\mathrm{C}}$$

where

$$R(T) = 4.27 \cdot 10^{26} \frac{T_{9,a}^{5/6}}{T_9^{3/2}} \exp\left[\frac{-84.165}{T_{9,a}^{1/3}} - 2.12 \cdot 10^{-3} T_9^3\right]$$

where $T_9 = T/10^9$ and $T_{9,a} = T_9/(1 + 0.0396 T_9)$

Energy release is $5.57 \cdot 10^{17} erg/g$

Studies

- Validation against FLASH code
- Landau-Darrieus instability
- Rayleigh-Taylor instability

Landau-Darrieus Instability

Multimode and single mode studies

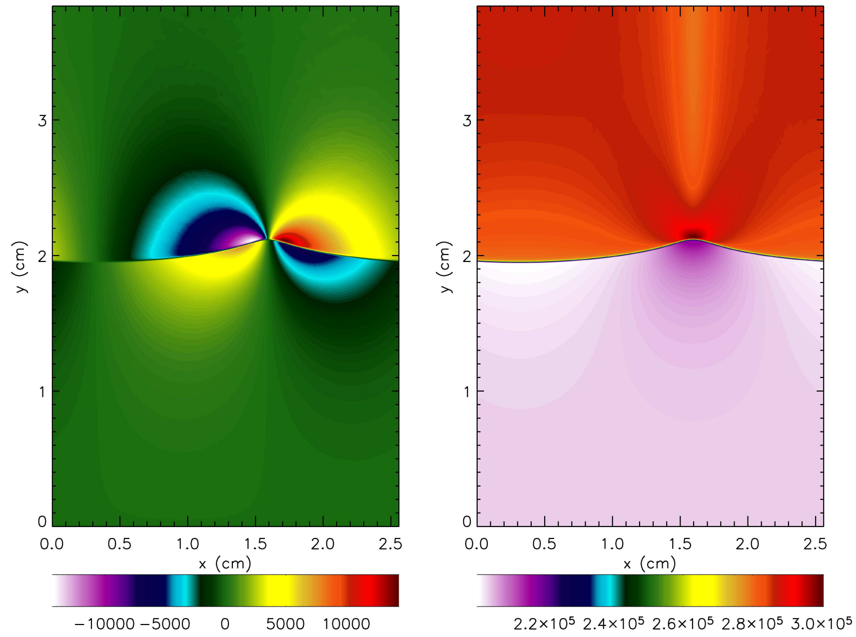
- Multimode perturbations gradually merge
- Range of densities ($2 \times 10^7$to 8×10^7 g cm-3)
- Varying domain width

Well defined cusps form and persist

- No breakdown in the non-linear regime observed.

Accelerations of a few % observed.

Curvature effects show $|Ma| \approx 2$ in agreement with compressible calculations of Dursi et al. (2003)

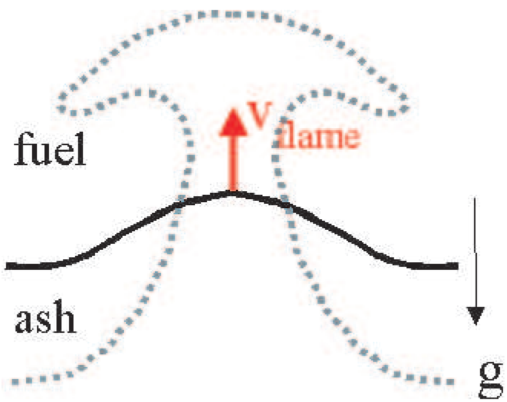


Interface Motion

Y-Velocity

Y-Velocity

Reactive Rayleigh=Taylor



$\rho_{ash} < \rho_{fuel}$

Rayleigh-Taylor

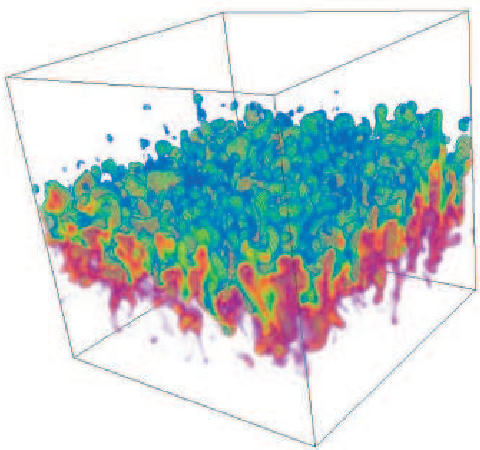
- Buoyancy driven instability.
- Large amounts of surface area generated.

Sharp-Wheeler model predicts mixed region growth

$$h = \alpha A g t^2$$

Reactions set a small scale cutoff to the growth to the instability:

$$\lambda_{fp} = 4\pi \frac{v_{laminar}^2}{g_{eff}}$$



Calder et al. (2002)

RT — Simulation Parameters

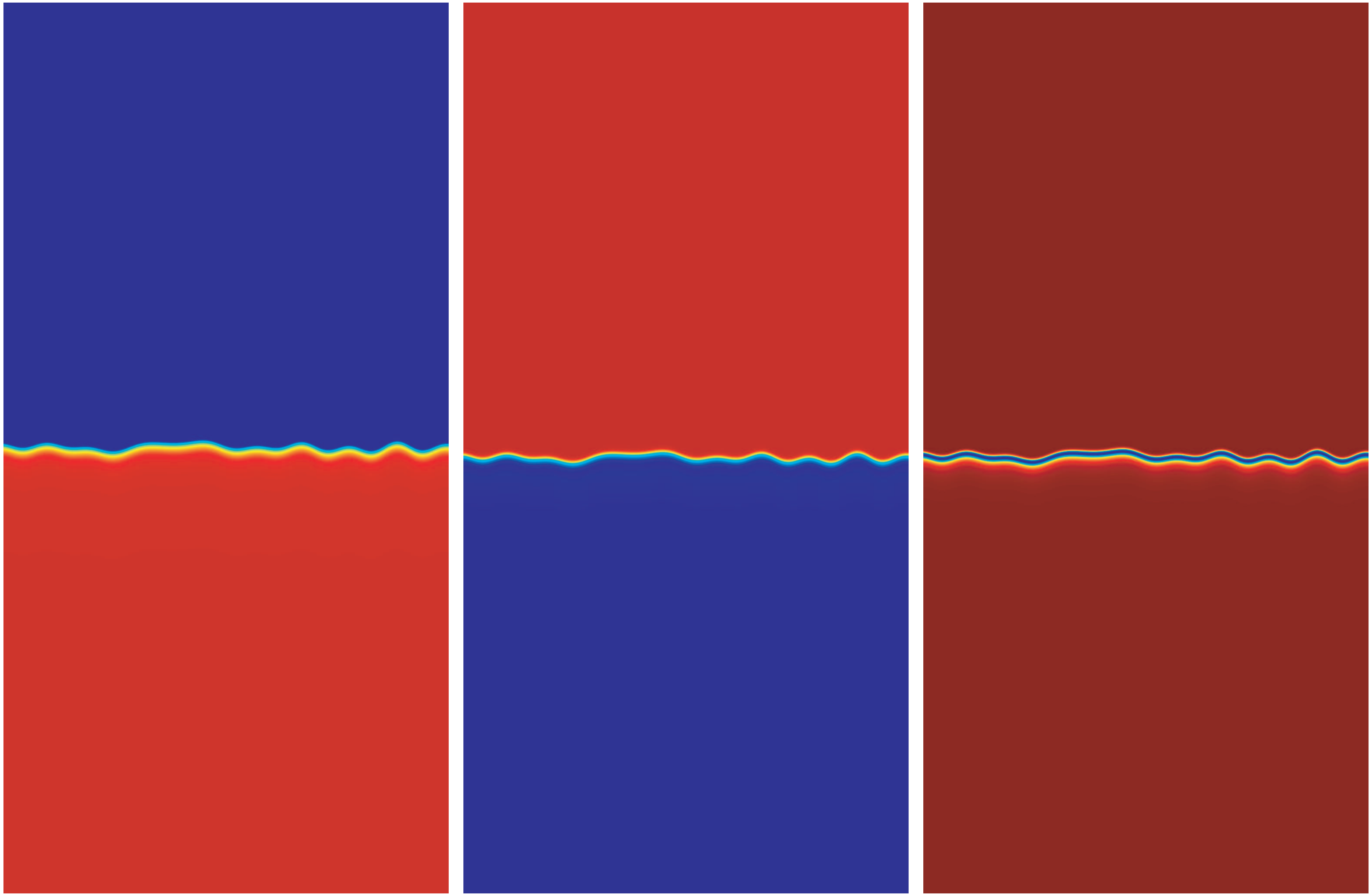
ρ (g cm^{-3})	$\Delta\rho/\rho$	v_{laminar} (cm s^{-1})	l_f [a] (cm)	λ_{fp} [b] (cm)	M
6.67×10^6	0.529	1.04×10^3	5.6	0.026	3.25×10^{-6}
10^7	0.482	2.97×10^3	1.9	0.23	8.49×10^{-6}
1.5×10^7	0.436	7.84×10^3	0.54	1.8	2.06×10^{-5}

Expansion $\approx 2\times$ behind the flame
Densities around $10^7\ g\ \ cm^{-3}$ pass through the region where

$$\lambda_{fp} = \ell_f$$

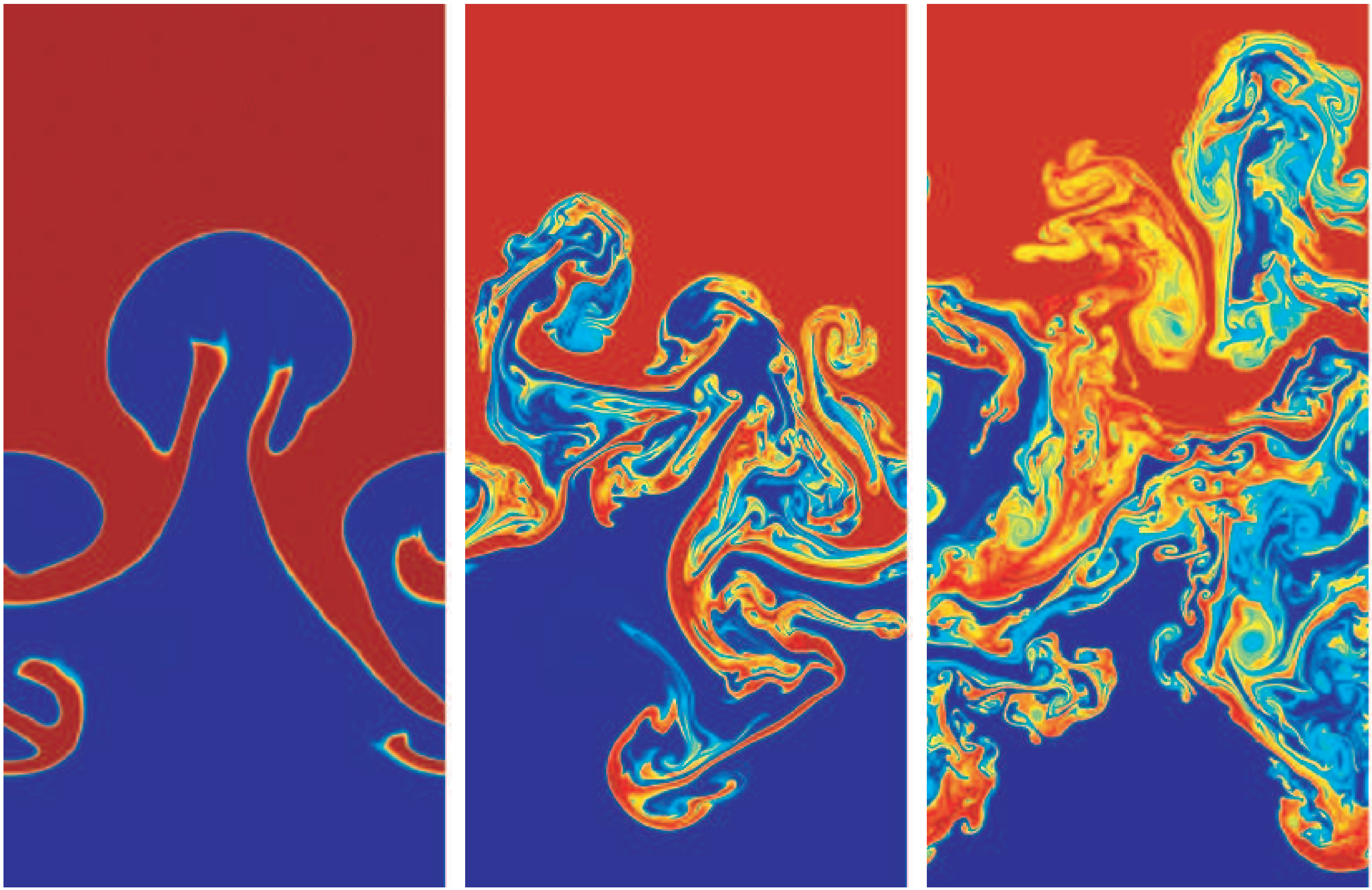
Transition to distributed burning predicted to occur at this density.
(Niemeyer and Woosley 1997)

Simulation results



Temperature Carbon Abundance Energy

Transition to distributed burning



Flame Acceleration / Growth

Effective flame speed increases of up to 6x are found

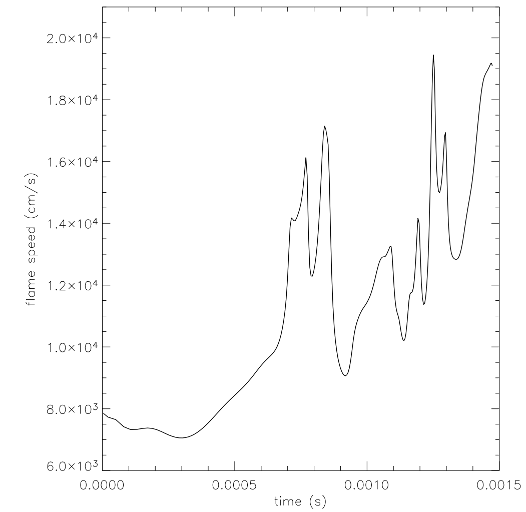
- Limited only by size of domain

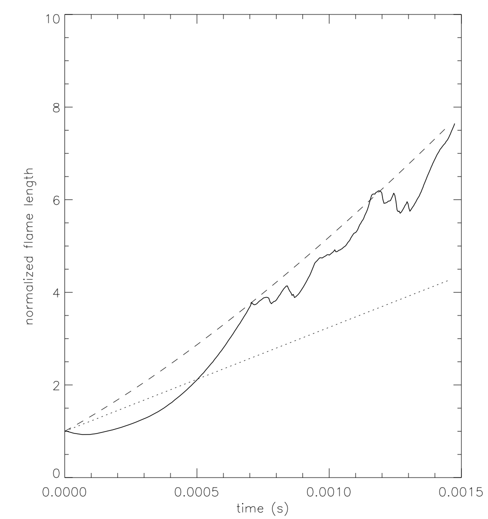
Flame length growth > acceleration

- Curvature effects
- Closer agreement to pure geometric scaling as density increases

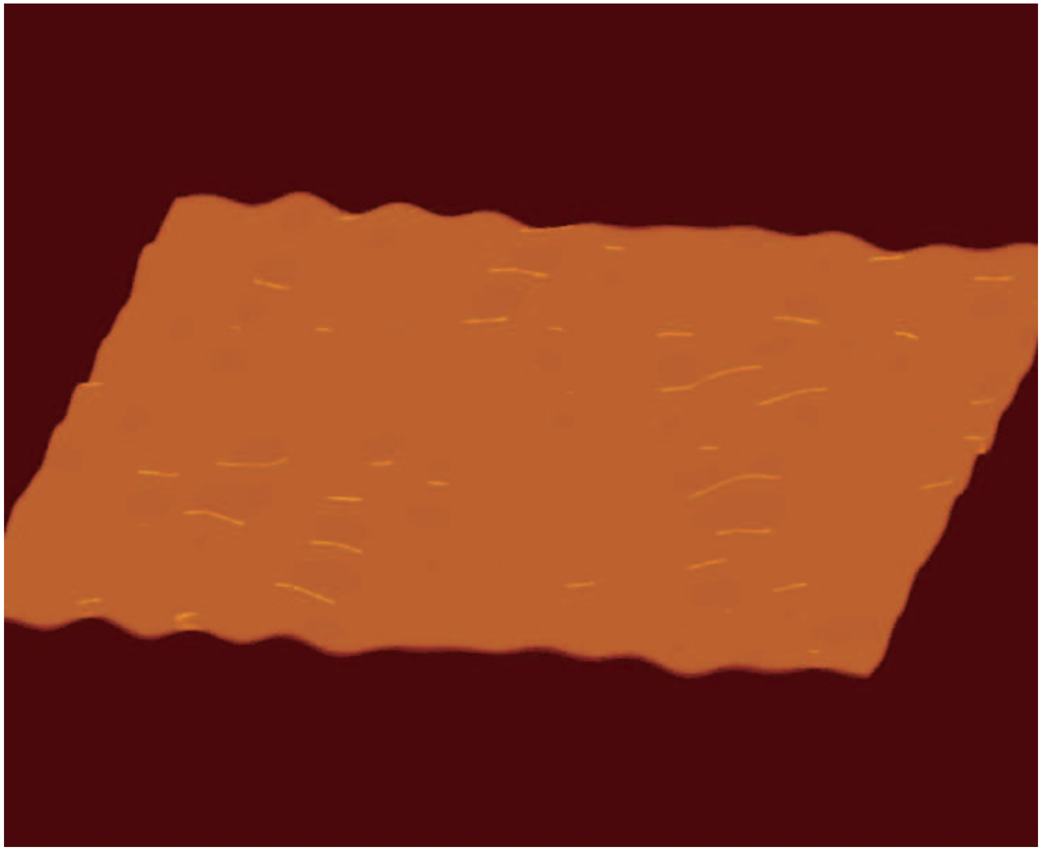
Flame growth follows power law scaling

$$L = L_0 \frac{\lambda_{max}}{\lambda_{min}}^{D-1} = L_) \left(\frac{\alpha g_{eff}^2 (t - t + 0)^2}{4 \pi v_{laminar}^2} \right)^{D-1}$$





3D Rayleigh Taylor



Flame surface – full system

Flame surface – zoom

Summary

Low Mach number methodology based on variable-ρ projection

- Conservative
- Second-order in time and space
- General equation of state
- Adaptive
- Parallel
- Application to nuclear flame microphysics
  - Landau Darrieus
  - Rayleigh Taylor
- Analysis 3-D Rayleigh-Taylor instability in supernovae
- 3D burning bubbles
- Modeling issues
  - Applicability and limitations of flamelet models
  - Appicability and linitations of thickened flame models